

> d his

(FILE 'HOME' ENTERED AT 14:09:36 ON 02 NOV 2005)

FILE 'REGISTRY' ENTERED AT 14:09:50 ON 02 NOV 2005

FILE 'CAPLUS' ENTERED AT 14:10:09 ON 02 NOV 2005

L1

STRUCTURE UPLOADED

S L1

FILE 'REGISTRY' ENTERED AT 14:10:42 ON 02 NOV 2005

L2

10 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:10:45 ON 02 NOV 2005

L3

11 S L2 FULL

L4

7 S L3 AND PY<2003

L5

0 S L4 AND ORTHORHOMBIC

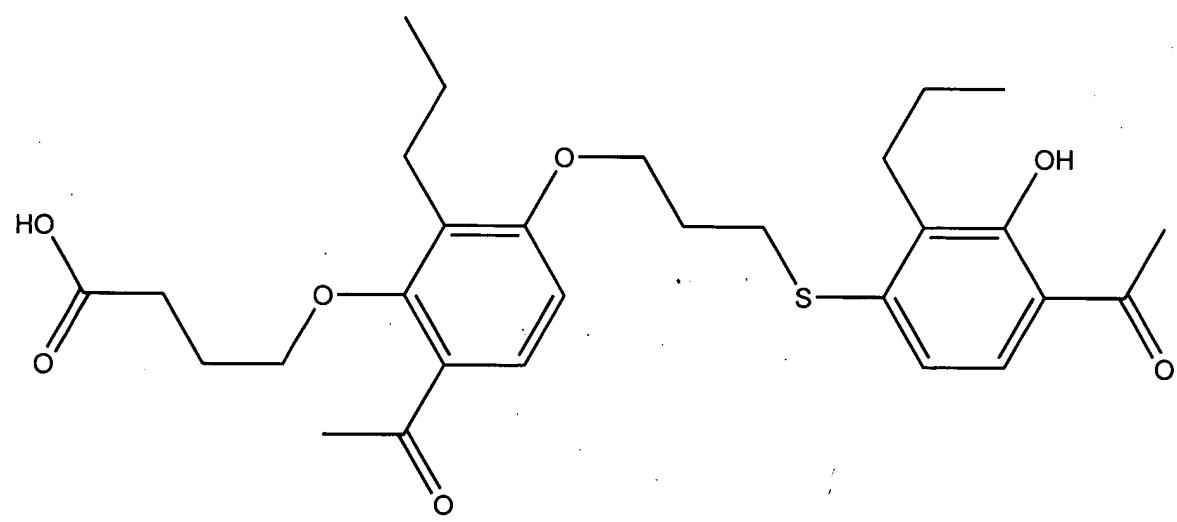
L6

0 S L4 AND CRYSTAL?

L7

0 S L4 AND POLYMORPH

=>



4-[6-ACETYL-3-[3-(4-ACETYL-3-HYDROXY-2-PROPYLPHENYLTHIO)PROPOXY]-2-PROPYLPHENOXY]BUTYRIC ACID

=> s 11 full
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 14:10:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 422943 TO ITERATE

100.0% PROCESSED 422943 ITERATIONS 10 ANSWERS
SEARCH TIME: 00.00.04

L2 10 SEA SSS FUL L1

L3 11 L2

=> s 13 and py<2003
22790221 PY<2003
L4 7 L3 AND PY<2003

=> s 14 and orthorhombic
59874 ORTHORHOMBIC
L5 0 L4 AND ORTHORHOMBIC

=> s 14 and crystal?
1695429 CRYSTAL?
L6 0 L4 AND CRYSTAL?

=> d 14 1-7 ibib abs hitstr

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:564826 CAPLUS
DOCUMENT NUMBER: 135:142249
TITLE: Eye drop compositions containing leukotriene antagonist KCA-757
INVENTOR(S): Kodaira, Hiromichi; Kozuka, Hitoshi
PATENT ASSIGNEE(S): Kyorin Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001054684	A1	20010802	WO 2001-JP430	20010124 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2397755	AA	20010802	CA 2001-2397755	20010124 <--
AU 2001028804	A5	20010807	AU 2001-28804	20010124 <--
EP 1250924	A1	20021023	EP 2001-946788	20010124 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
TW 526061	B	20030401	TW 2001-90101616	20010129

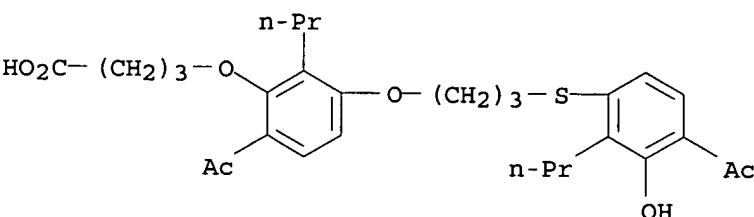
US 2003083378 A1 20030501 US 2002-181436 20020725
 PRIORITY APPLN. INFO.: JP 2000-17403 A 20000126
 WO 2001-JP430 W 20010124

AB Disclosed are eye drops containing a potent and selective leukotriene antagonist. Specifically, stable eye drops of an aqueous solution or suspension type, containing as the active ingredient 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-propylphenoxy]butyric acid (KCA-757). An eye drop composition containing KCA-757 0.5 g, 0.1 M NaOH 20 mL, potassium dihydrogenphosphate 0.004, sodium hydrogenphosphate 0.089, NaCl 0.8 g, and 0.1 M HCl q.s. to pH 8.5, and water q.s. to 100 mL was formulated.

IT 125961-82-2
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (eye drop compns. containing leukotriene antagonist KCA-757)

RN 125961-82-2 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-propylphenoxy] - (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1999:205557 CAPLUS
 DOCUMENT NUMBER: 130:287054
 TITLE: Powder inhalants containing [(propylphenyl)thio]propoxypropylphenoxybutyrate for the treatment of asthma
 INVENTOR(S): Hoshino, Ryoichi
 PATENT ASSIGNEE(S): Kyorin Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

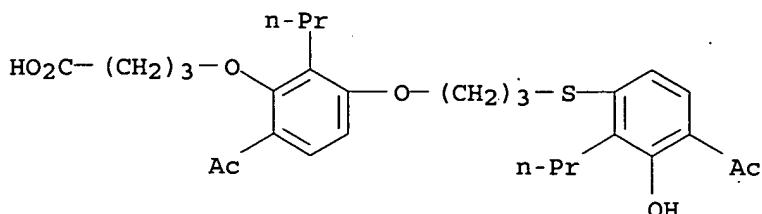
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11079985	A2	19990323	JP 1997-251280	19970901 <--
			JP 1997-251280	19970901

PRIORITY APPLN. INFO.: AB Powder inhalants for the treatment of asthma comprise powdery 4-[6-acetyl-3-[3-(4-acetyl-3-hydroxy-2-propylphenylthio)propoxy]-2-propylphenoxy]butyric acid (I) as an active ingredient. I in combination with lubricants is suspended in an aqueous solution of polymers and spray dried to give a fine powder having an average particle diam \leq 6 μ m. The powders show little self-cohesive properties and little adhesion to a dispersing device. Hydroxypropyl Me cellulose 1.5 g was dissolved in 380 g distilled water and to the solution 0.5 g sucrose fatty acid ester was added, followed by 18 g I. The dispersion was subjected to a high-pressure homogenization and spray-drying to give a dry powder inhalant.

IT 125961-82-2
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (manufacture of antiasthmatic powder inhalants containing [(propylphenyl)thiopropoxy]propylphenoxybutyrate and polymers and lubricants)

RN 125961-82-2 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-propylphenoxy]- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:379374 CAPLUS

DOCUMENT NUMBER: 125:58104

TITLE: Preparation of phenoxycarboxylic acid derivatives as antiallergy agents

INVENTOR(S): Matsumoto, Toyomi; Ishiguro, Juji; Myashita, Kunio; Kitamura, Genichi

PATENT ASSIGNEE(S): Kyorin Seiyaku Kk, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

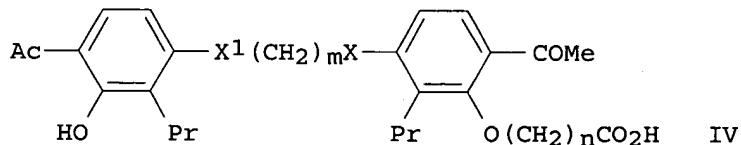
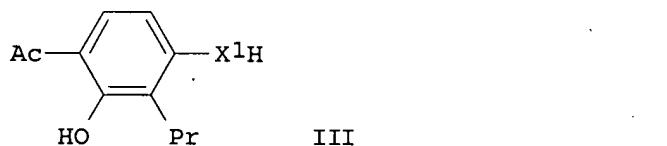
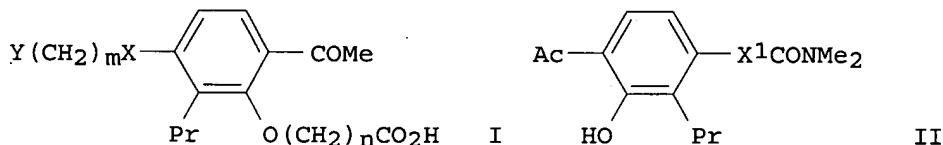
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08081412	A2	19960326	JP 1994-244636	19940913 <--
PRIORITY APPLN. INFO.:			JP 1994-244636	19940913
OTHER SOURCE(S):	CASREACT 125:58104; MARPAT 125:58104			
GI				



AB The title derivs. IV ($m = 2-5$; $n = 3-8$; $X_1 = S, O; X = O, S, SO, SO_2; X_1 = X \neq O$), useful as antiallergy agents (no data), are prepared by treating phenoxycarboxylic acids I ($Y = \text{halo}$) with hydroxybenzenes III, which is formed by hydrolysis of hydroxyphenyl carbamates II, in one pot. A mixture of 10 g $S-(4\text{-acetyl-3-hydroxy-2-propylphenyl})N,N\text{-dimethylthiocarbamate}$ and KOH in H₂O was treated at 95° for 1.5 h, then treated with 12.7 g 4-[6-acetyl-3-hydroxy-3-(3-chloropropoxy)-2-propylphenoxy]butyric acid at 35-40° for 21 h to give 15.2g 4-[6-acetyl-3-(3-(4-acetyl-3-hydroxy-2-propylphentylthio)propoxy)-2-

IT propylphenoxy]butyric acid.

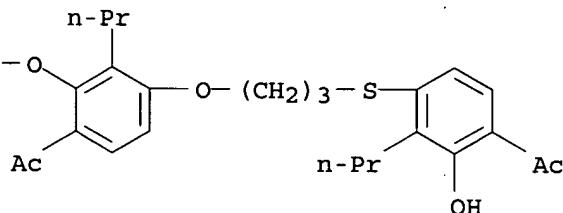
125961-82-2P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of phenoxy carboxylic acid as antiallergy agent from phenoxy carboxylate and hydroxyphenyl carbamate)

RN 125961-82-2 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thiol]propoxy]-2-propylphenoxy] - (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:403614 CAPLUS

DOCUMENT NUMBER: 122:290448

TITLE: Preparation of (acetylpropylphenoxy)alkanoic acids as intermediates for antiallergic leukotriene antagonists

INVENTOR(S): Matsumoto, Toyomi; Aizawa, Yasuhiro; Matsukubo, Hiroshi

PATENT ASSIGNEE(S): Kyorin Seiyaku Kk, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

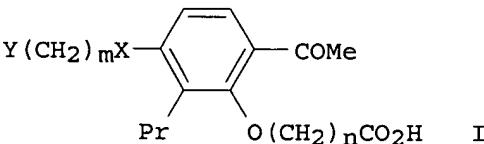
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06345682	A2	19941220	JP 1993-166354	19930611 <-
PRIORITY APPLN. INFO.:			JP 1993-166354	19930611
OTHER SOURCE(S):	MARPAT	122:290448		

GI



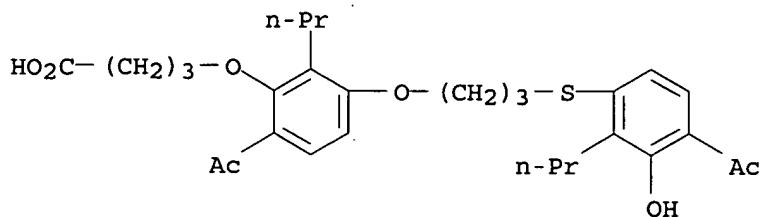
AB The title compds. I ($m = 2-5$; $n = 3-8$; X = O, S, SO, SO2; Y = halo) are claimed. An aqueous NaOH solution was added dropwise to an EtOH solution of 4-[6-acetyl-3-(3-chloropropoxy)-2-propylphenoxy]butyric acid Et ester (preparation given) at 18-28° and the reaction mixture was stirred at room temperature for 2 h to give 91% 4-[6-acetyl-3-(3-chloropropoxy)-2-propylphenoxy]butyric acid (II). II (21.4 g) and 15.1 g 2-hydroxy-4-mercaptopropanoate were dissolved in DMF and the solution was treated with K2CO3 under stirring at room temperature for 3 h to give 24.4 g 4-[6-acetyl-3-[3-(4-acetyl-3-hydroxy-2-propylphenylthio)propoxy]-2-propylphenoxy]butyric acid as a leukotriene antagonist.

IT 125961-82-2P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of (acetylpropylphenoxy)alkanoic acids as intermediates for leukotriene antagonists)

RN 125961-82-2 CAPLUS
 CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-propylphenoxy]- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:39068 CAPLUS

DOCUMENT NUMBER: 123:169347

TITLE: preparation of phenylthiopropoxyphenyloxybutyric acid derivatives as leukotriene antagonists

INVENTOR(S): Oohashi, Mitsuo; Hori, Wataru

PATENT ASSIGNEE(S): Kyorin Seiyaku Kk, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

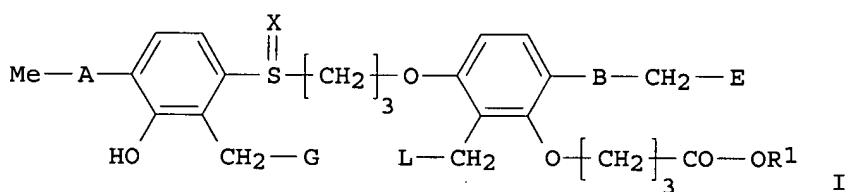
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06100526	A2	19940412	JP 1992-273717	19920917 <--
PRIORITY APPLN. INFO.:			JP 1992-273717	19920917
OTHER SOURCE(S):	MARPAT	123:169347		
GI				



AB Title derivs. I (A, B = CO, hydroxymethylene; E = H, OH, acetoxy; G, L = Et, acetyl, 1-hydroxyethyl, 2-hydroxyethyl, hydroxycarbonylmethyl, lower alkoxy carbonylmethyl; X = void, O, O2; R1 = H, lower alkyl; X = O, O2 and B = hydroxymethylene when A = carbonyl, E = H, and G = L = Et) or their alkali salts, acting as strong antagonists for leukotrienes C4, D4, and E4 and useful for antiasthmatics, are prepared. Thus, treating 2'-hydroxy-3'-(2-hydroxypropyl)-4'-mercaptoacetophenone (prepared in 6 steps from 3-allyl-2,4-dihydroxyacetophenone) with Et 4-[6-acetyl-3-(3-bromopropoxy)-2-propylphenoxy]butyrate gave I (A = B = CO, E = H, G = 1-hydroxyethyl, L = Et, R1 = Et, X = void).

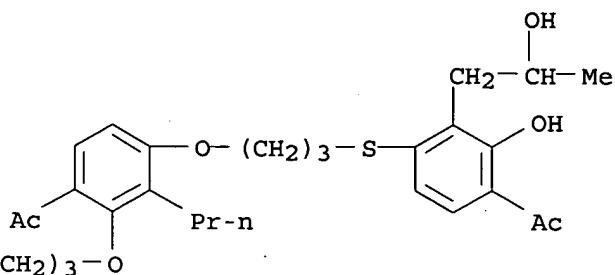
IT 167211-62-3P 167211-73-6P 167211-79-2P

167211-83-8P 167211-94-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of phenylthiopropoxyphenyloxybutyric acid derivs. as leukotriene antagonists)

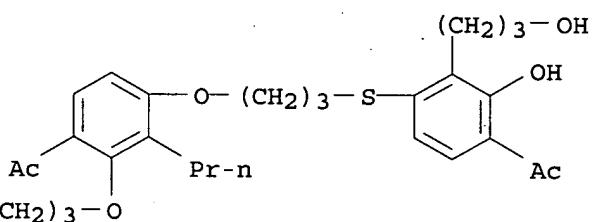
RN 167211-62-3 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-(2-hydroxypropyl)phenyl)thio]propoxy]-2-propylphenoxy]- (9CI) (CA INDEX NAME)



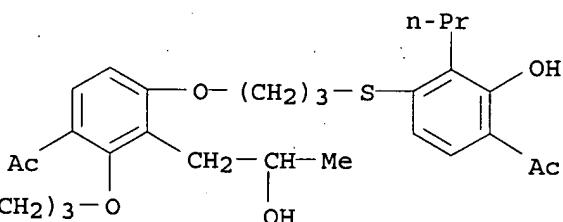
RN 167211-73-6 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-(3-hydroxypropyl)phenyl]thio]propoxy]-2-propylphenoxy]- (9CI) (CA INDEX NAME)



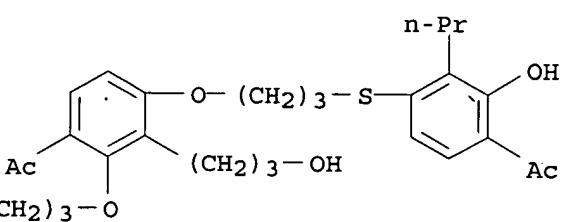
RN 167211-79-2 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-(2-hydroxypropyl)phenoxy]- (9CI) (CA INDEX NAME)



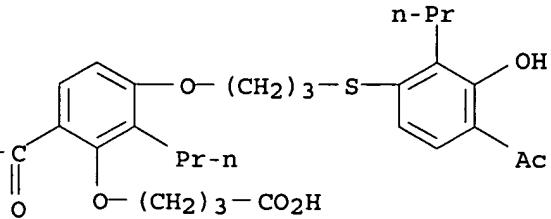
RN 167211-83-8 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-(3-hydroxypropyl)phenoxy]- (9CI) (CA INDEX NAME)



RN 167211-94-1 CAPLUS

CN Butanoic acid, 4-[3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-6-(hydroxyacetyl)-2-propylphenoxy]- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:138760 CAPLUS

DOCUMENT NUMBER: 112:138760

TITLE: Preparation of phenoxyalkylcarboxylic acid derivatives as antiallergic agents

INVENTOR(S): Ohashi, Mitsuo; Awano, Katsuya; Tanaka, Toshio; Kimura, Tetsuya

PATENT ASSIGNEE(S): Kyorin Pharmaceutical Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 32 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

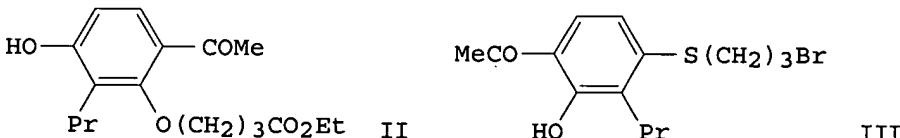
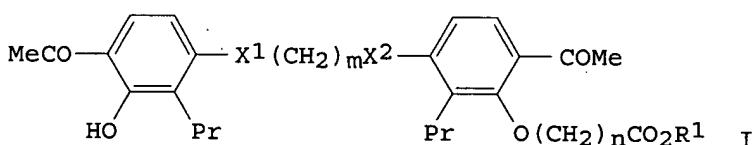
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 332109	A1	19890913	EP 1989-103897	19890306 <--
EP 332109	B1	19911204		
R: BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
JP 02001459	A2	19900105	JP 1989-38912	19890218 <--
JP 07116125	B4	19951213		
US 4985585	A	19910115	US 1989-313900	19890223 <--
AU 8930884	A1	19890907	AU 1989-30884	19890301 <--
AU 617439	B2	19911128		
CA 1331763	A1	19940830	CA 1989-592555	19890302 <--
HU 50112	A2	19891228	HU 1989-1039	19890303 <--
HU 204030	B	19911128		
HU 208418	B	19931028	HU 1991-2410	19890303 <--
HU 208524	B	19931129	HU 1991-2411	19890303 <--
ES 2045219	T3	19940116	ES 1989-103897	19890306 <--
CN 1036560	A	19891025	CN 1989-101301	19890307 <--
CN 1022407	B	19931013		

PRIORITY APPLN. INFO.: JP 1988-53374 A 19880307
HU 1989-1039 A3 19890303

OTHER SOURCE(S): MARPAT 112:138760

GI



AB The title compds. (I; R1 = H, Me, Et; X1, X2 = O, S, SO, SO2; X1 = X2 ≠ O; m = 2-5; n = 3-8), useful as antiallergic agents, are prepared. A mixture of phenoxybutyrate II, bromopropyl thioether III, KI, and K2CO3 in

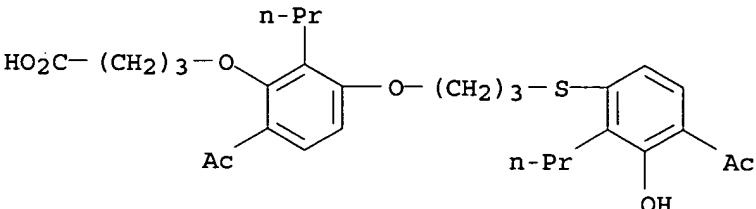
Me₂CO was refluxed to give 72.4% I (R₁ = Et, X₁ = S, X₂ = O, m = n = 3). I showed 66.7-96.2% inhibition of leukotriene D₄-induced bronchoconstriction at 50 mg/kg p.o. in guinea pigs. Addnl. 70 I were also prepared

IT 125961-82-2P 125961-92-4P 125961-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as antiallergic agent)

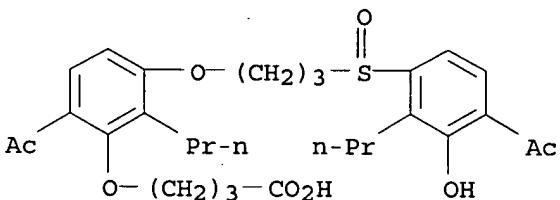
RN 125961-82-2 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-propylphenoxy] - (9CI) (CA INDEX NAME)



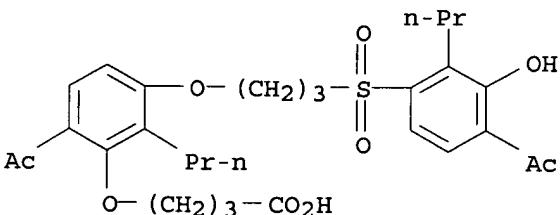
RN 125961-92-4 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)sulfinyl]propoxy]-2-propylphenoxy] - (9CI) (CA INDEX NAME)



RN 125961-93-5 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)sulfonyl]propoxy]-2-propylphenoxy] - (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1983:575604 CAPLUS

DOCUMENT NUMBER: 99:175604

TITLE: Anti-SRS-A carboxylic acid derivatives and pharmaceutical formulations containing them

INVENTOR(S): Bantick, John Raymond

PATENT ASSIGNEE(S): Fisons Ltd., UK

SOURCE: Eur. Pat. Appl., 67 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

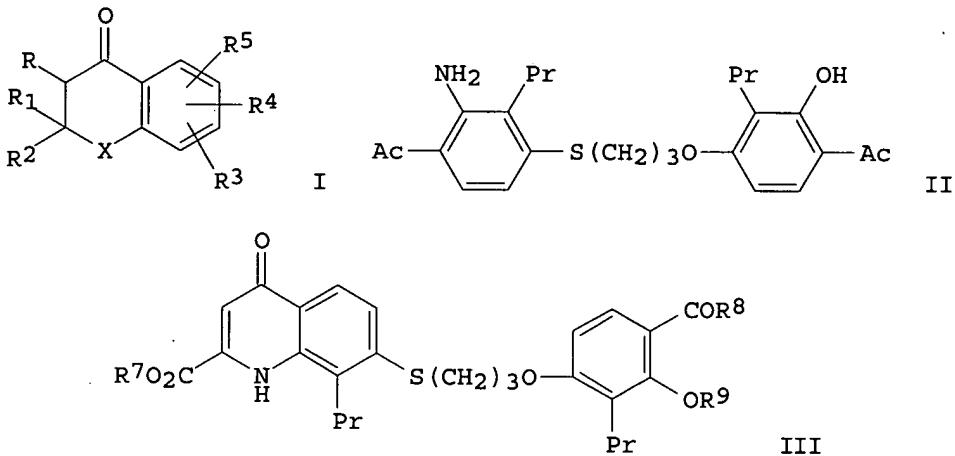
KIND DATE

APPLICATION NO.

DATE

EP 79637	A1	19830525	EP 1982-201368	19821101 <--
EP 79637	B1	19870128		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4474788	A	19841002	US 1982-438163	19821101 <--
AT 25251	E	19870215	AT 1982-201368	19821101 <--
JP 58090557	A2	19830530	JP 1982-196883	19821111 <--
PRIORITY APPLN. INFO.:				
			GB 1981-34186	A 19811112
			EP 1982-201368	A 19821101

GI



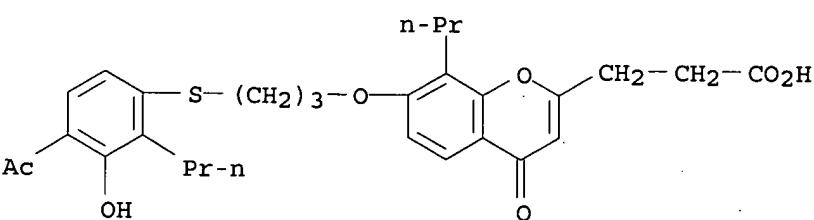
AB Anti-allergy (no data) bicyclic compds. I [R, R1 = H, alkyl; RR1 = bond; R2 = CO2H, carboxyalkyl; R3 = substituted OH, SH, NH2; R4, R5 = H, halogen, (un)substituted OH, NH2, alkyl, acyl; X = S, O, NR6 (R6 = H, alkyl)] were prepared. Thus, 3,2,4-Pr(HO)2C6H2Ac reacted with 4,2,3-AcPr(H2N)C6H2S(CH2)3Br to give phenol II, which cyclized with EtO2CCO2Et to give quinoline III [R7 = Et, R8R9 = CH:C(CO2Et)]. The latter compound gave III (R7 = H, R8 = Me, R9 = H) on hydrolysis.

IT 87472-35-3P 87472-36-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 87472-35-3 CAPLUS

CN 4H-1-Benzopyran-2-propanoic acid, 7-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-4-oxo-8-propyl- (9CI) (CA INDEX NAME)



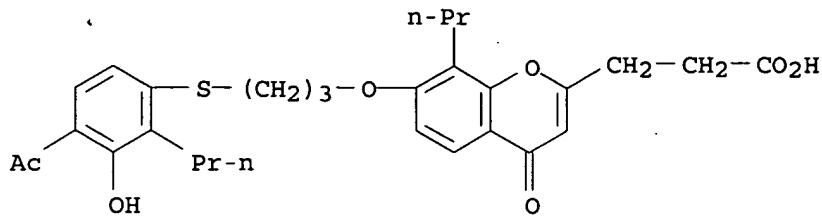
RN 87472-36-4 CAPLUS

CN L-Lysine, mono[7-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-4-oxo-8-propyl-4H-1-benzopyran-2-propanoate] (9CI) (CA INDEX NAME)

CM 1

CRN 87472-35-3

CMF C29 H34 O7 S



CM 2

CRN 56-87-1
CMF C6 H14 N2 O2

Absolute stereochemistry.

